Electronic states on a twin boundary of a d-wave superconductor

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We show that an induced s-wave harmonic in the superconducting gap of an orthorhombic $d_{x^2-y^2}$ superconductor strongly affects the excitation spectrum near a twinning plane. In particular, it yields bound states of zero energy with areal density proportional to the relative weight of the s-wave component. An unusual scattering process responsible for the thermal conductivity across the twin boundary at low temperatures is also identified.

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The controversy concerning s-wave versus d-wave pairing in high-T_c superconductors is being gradually resolved in favor of the $d_{x^2-y^2}$ symmetry. This is possible because of precise measurements of spontaneously generated half-integral flux quanta on bicrystal and tricrystal films [1] together with the corner SQUID experiments [2], which all suggest that the superconducting gap changes sign on the Fermi surface between the a- and b-directions with zeros or nodes in between. The existence of corresponding low-energy excitations in the superconducting state of cuprates have also been demonstrated by measurements of the magnetic penetration depth [3], the nuclear spin relaxation rate [4], and by angular resolved photoemission data [5].

However, not all experimental data fit into a simple picture of a pure $d_{x^2-y^2}$ order parameter. Sun *et al.* [6] have found a non-vanishing tunneling current along the c-axis between $YBa_2Ca_3O_{6+x}$ (YBCO) and the conventional superconductor Pb, which cannot exist for a tetragonal d-wave superconductor. It was argued [7,8] that such an experiment can be understood if an admixture of an s-wave component due to the orthorhombicity of YBCO crystals [9] is taken into account. The mixed wave $d{+}s$ gap then has nodes on the Fermi surface shifted from the principal diagonal directions. Recent high resolution measurements of the ab-plane thermal conductivity have failed to see this effect imposing an upper limit of 10% on the weight of the s-wave harmonic [10].

An important challenge for current research is to reconcile various conflicting results on symmetry of the superconducting order parameter in YBCO by direct determination of the s-wave component in the gap. In this work we study the structure of the quasiparticle spectrum close to a twinning plane in a predominantly d-wave orthorhombic superconductor and show that it changes significantly in the presence of an s-wave component of the gap. In particular, there appear bound states of zero energy with areal density proportional to the magnitude of the s-wave component. Bound states cause a modification of the local density of states which can be observed by scanning tunneling microscopy. Other new effects studied below include an unusual low temperature mechanism of heat transport across the twin boundaries. This is a kind of Andreev transmission process because it involves particle-hole conversion.

The tetragonal symmetry of the CuO_2 planes in YBCO is spoiled by the presence of CuO chains. The two possible orientations of the chains lead to the formation of so-called twin domains separated by twin boundaries (TBs), which are (110) or $(1\bar{1}0)$ planes of the original tetragonal lattice (Fig 1). The structural anisotropy gives rise to an anisotropy in the pairing interaction and, hence, to an admixture (real combination) of s- and d-waves in the superconducting gap with the relative phase 0 or π in different twins [9]. Since we assume the dominant component of the gap to be of the d-wave symmetry, a natural energy requirement is that ψ_d stays almost constant across the boundary, whereas ψ_s has different signs on both sides, thus exhibiting a soliton-like structure. The symmetry of the combined order parameter ($d \pm s$) is, in this case, odd with respect to the reflection in the twinning plane. Note, that the opposite assumption of an even symmetry state ($s \pm d$) is in conflict with the ab-tunneling experiments on heavily twinned YBCO samples [8]. Sigrist and co-workers [7] suggested that the s-wave component could change sign between two twin domains by avoiding zero at the twin boundary and forming a time-reversal breaking state $d + se^{i\chi}$. Existence of the time-reversal breaking states on twin boundaries in YBCO is still an open question, we therefore leave discussion of the electronic spectrum for such a twin boundary to the end.

The soliton-like behavior of the induced s-wave component plays a key role in the formation of bound states on twin boundaries. Examples of fermions trapped on one-dimensional inhomogeneities of the off-diagonal potential have been known for a long time [11]. To get some insight into this we first consider a very simplified model of the boundary between two twins. Namely, we neglect all orthorhombic effects except the induced inhomogeneous s-wave component and assume cylindrical Fermi surface. The Bogoliubov-de Gennes (BdG) equations in the quasiclassical approximation [12], i.e., retaining terms of the

lowest order in $(k_F\xi_0)^{-1}$, are written for a slowly varying function of space coordinates $(u,v)=e^{-i\mathbf{k}_F\cdot\mathbf{r}}\psi$, ψ being the usual BdG wave function, as

$$E\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} -i\mathbf{v}_F\cdot\boldsymbol{\nabla} & \Delta(\mathbf{k}_F,\mathbf{r}) \\ \Delta^*(\mathbf{k}_F,\mathbf{r}) & i\mathbf{v}_F\cdot\boldsymbol{\nabla} \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}, \qquad (1)$$

where $\mathbf{v}_F=\mathbf{k}_F/m$ ($\hbar=1$). For the pair potential close to the twin boundary ($x=0$ plane) we choose

$$\Delta(\mathbf{k},\mathbf{r})=\Delta_d(\mathbf{k})+\Delta_s\tanh(x/\xi_0)\ , \qquad (2)$$

which gives correct orthorhombic gaps $\Delta_d\pm\Delta_s$ at $x\to\pm\infty$. At $E=0$, system (1) can be transformed to a pair of independent first-order differential equations, which are easily solved giving

$$\psi_+ = Ce^{i\mathbf{k}_F\cdot\mathbf{r}}e^{-x/\xi_d}\frac{1}{[\cosh(x/\xi_0)]^{\xi_0/\xi_s}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$
$$\psi_- = Ce^{i\mathbf{k}'_F\cdot\mathbf{r}}e^{x/\xi_d}\frac{1}{[\cosh(x/\xi_0)]^{\xi_0/\xi_s}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \qquad (3)$$

where $\mathbf{k}'_F=(-k_{Fx},k_{Fy})$, $\Delta_d(\mathbf{k}'_F)=-\Delta_d(\mathbf{k}_F)$, $\xi_d=v_{Fx}/|\Delta_d(\mathbf{k}_F)|$, $\xi_s=v_{Fx}/\Delta_s$. These solutions correspond to physical states whenever normalization condition can be satisfied. Since the asymptotic behavior of ψ does not depend on ξ_0, we immediately conclude that the bound state for a given $\mathbf{k}_F$ exists if $\Delta(\mathbf{k}_F,\infty)$ and $\Delta(\mathbf{k}_F,-\infty)$ have *different* signs, e.g., for $k_{y\mathrm{C}'}<k_{Fy}<k_{y\mathrm{A}}$ in Fig. 2. This requirement can also be written as $|\Delta_d(\mathbf{k}_F)|<\Delta_s$. For a model d-wave gap $\Delta_d(\mathbf{k})=\Delta_0(k_a^2-k_b^2)/k_F^2$ or, in our coordinate system, $\Delta_d(\mathbf{k})=2\Delta_0k_xk_y/k_F^2$, the midgap excitations exist in the vicinity of $(\pm k_F,0)$ for $|k_y|<(\Delta_s/2\Delta_0)k_F$ and close to $(0,\pm k_F)$ with the same condition on k_x, though in the latter case, as we shall see below, these states are easily destroyed by various perturbations.

The local density of states near the twin boundary has a δ-like peak at $E=0$ corresponding to the bound states. The associated areal density

$$N_B(E)=\delta(E)\sum_n\int|v_n^b(x)|^2dx=\frac{2k_F}{\pi}\frac{\Delta_s}{\Delta_0}\delta(E) \qquad (4)$$

is proportional to the relative weight of the s-wave component. Furthermore, it is possible to show with the help of the Atiyah-Singer theorem that the zero-energy branch found for the gap function (2) exists for a wide class of gaps between two twins [13].

To describe more realistically anisotropy of electron properties in YBCO we now consider a second model, which is a tight-binding model of a single CuO_2 plane. The model includes the orthorhombicity through unequal effective hopping matrix elements t_1 and t_2 along the a and b axes. The two different hopping amplitudes allow us to construct a twinning plane on a square lattice as shown in Fig. 1. An extra local potential (which we denote by U_0 and assume positive) associated with atoms on the twin boundary is allowed by the symmetry and will be shown to have important consequences for the twin boundary properties. Thus, the one-electron Hamiltonian of the normal phase is

$$\hat{H}_0=\sum_{ij\sigma}(t_{ij}-\mu\delta_{ij})c^\dagger_{i\sigma}c_{j\sigma}+U_0\sum_{i\in\mathrm{TB}\sigma}c^\dagger_{i\sigma}c_{i\sigma}\ . \qquad (5)$$

The Schrödinger equation for the discrete function $\psi_{i\sigma}$ is

$$(E+\mu)\psi_{i\sigma}=\sum_j t_{ij}\psi_{j\sigma}+U_0\psi_{i\sigma}|_{i\in\mathrm{TB}}\ . \qquad (6)$$

The dispersions of plane waves in the two twins are

$$\varepsilon(\mathbf{k})=-2(t_{1,2}\cos k_a+t_{2,1}\cos k_b)-\mu$$
$$=-4t\cos\frac{k_x}{\sqrt{2}}\cos\frac{k_y}{\sqrt{2}}\mp4t\epsilon\sin\frac{k_x}{\sqrt{2}}\sin\frac{k_y}{\sqrt{2}}-\mu\ , \qquad (7)$$

where $t_{1,2}=t(1\pm\epsilon)$, and the lattice constant is taken to be unity.

Quasiparticles scatter on the twin boundary preserving their energy and the parallel component of their momentum. To study the scattering process we first find from Eq. (7) normal components of the Fermi momenta for incoming and outgoing electrons with a given parallel component k_y (see Fig. 2). In the right twin they are $k^>_{\pm x}=\pm k+q$, while in the left twin $k^<_{\pm x}=\pm k-q$,

$$\tan\frac{q}{\sqrt{2}}=\epsilon\tan\frac{k_y}{\sqrt{2}}\ , \qquad \cos\frac{k}{\sqrt{2}}=\frac{-\mu\cos(q/\sqrt{2})}{4t\cos(k_y/\sqrt{2})}\ . \qquad (8)$$

The normal components of the Fermi velocities for all these states have, however, the same absolute value $v_{Fx}=2\sqrt{2}t\sin(k/\sqrt{2})\cos(k_y/\sqrt{2})/\cos(q/\sqrt{2})$. (Note, that velocities are defined with dimension of energy.)

The wave function describing the scattering of an electron approaching the twin boundary from the right is

$$\psi^>_i=e^{i\mathbf{k}^>_-\cdot\mathbf{r}_i}+re^{i\mathbf{k}^>_+\cdot\mathbf{r}_i}\ (x>0), \quad \psi^<_i=de^{i\mathbf{k}^<_-\cdot\mathbf{r}_i}\ (x<0). \qquad (9)$$

Two equations for the unknown amplitudes r and d are (i) continuity of the wave function $\psi^>_0=\psi^<_0$ and (ii) Eq. (6) for $x=0$, which we write, after some algebra and Fourier transformation over y, as

$$\psi^>_1e^{-iq/\sqrt{2}}-\psi^<_1e^{iq/\sqrt{2}}=\frac{U_0\cos(q/\sqrt{2})}{2t\cos(k_y/\sqrt{2})}\psi_0\ . \qquad (10)$$

Remarkably, if $U_0=0$, quasiparticles move across the twinning plane without scattering for arbitrary degree of orthorhombicity ϵ. The potential barrier on the boundary yields a nonzero probability of the reflection with amplitude $r=\alpha/(i-\alpha)$, $\alpha=U_0/\sqrt{2}v_{Fx}$.

Below T_c we again will not attempt to solve the problem self-consistently but rather use a "guess" order parameter to study qualitative features of the quasiparticle spectrum. The discrete BdG equations are

$$E\psi_i = \sum_j \begin{pmatrix} t_{ij} - \mu\delta_{ij} & \Delta_{ij} \\ \Delta^*_{ij} & -t_{ij} + \mu\delta_{ij} \end{pmatrix} \psi_j \ , \qquad (11)$$

where ψ stands now for a vector with quasielectron and quasihole components. For orthorhombic symmetry and nearest-neighbor interactions we define $\Delta_{i\,i\pm a} = \Delta_1/2$, $\Delta_{i\,i\pm b} = -\Delta_2/2$ in one twin and $\Delta_{i\,i\pm a} = \Delta_2/2$, $\Delta_{i\,i\pm b} = -\Delta_1/2$ in the other, $\Delta_{1,2} = \Delta(1 \pm \delta)$ (see Fig. 1). The superconducting gap in the two twins is given by Fourier transform of the off-diagonal element in (11):

$$\Delta(\mathbf{k}) = \Delta(\cos k_a - \cos k_b) \pm \Delta\delta(\cos k_a + \cos k_b) \ . \quad (12)$$

A nonzero parameter δ describes effect of crystal orthorhombicity on superconducting properties and determines a relative weight of the s-wave component.

In our model of the twin boundary the first term of Eq. (12), i.e., the d-wave component, is chosen to be constant, whereas the second, extended s-wave part has a discontinues change of sign at the twinning plane. Although this assumption is not correct and Δ_s varies on a characteristic scale $\xi_s \gg a$, the qualitative picture remains the same since the discussed results depend only on the asymptotes of the order parameter. In the following analysis we will use the symmetry of the problem coming from relations $t_{\hat\sigma i \hat\sigma j} = t_{ij}$ and $\Delta_{\hat\sigma i \hat\sigma j} = -\Delta_{ij}$, where $\hat\sigma$ is reflection in the twinning plane. The BdG equations are invariant under the combined transformation $\hat U = \tau_3\hat\sigma$, τ_3 being the Pauli matrix which acts in the particle-hole space. All solutions of Eqs. (11) are, hence, classified by their parity with respect to $\hat U$.

In the bulk of each twin, Eqs. (11) are diagonalized by a transformation to plane waves. The wave function of a bound state is their linear combination

$$\psi_i^> = \begin{pmatrix} \Delta_- \\ E + i\Omega_- \end{pmatrix} e^{i\mathbf{k}_-\cdot\mathbf{r}_i - \kappa_- x} + R \begin{pmatrix} \Delta_+ \\ E - i\Omega_+ \end{pmatrix} e^{i\mathbf{k}_+\cdot\mathbf{r}_i - \kappa_+ x}$$

$$\Omega_\pm = \sqrt{\Delta_\pm^2 - E^2} \ , \quad \kappa_\pm = \Omega_\pm / v_{Fx} \qquad (13)$$

for $x > 0$, while on the left side $\psi_i^<$ for even and odd eigenfunctions are obtained from $\psi_i^< = \pm\tau_3\psi^>_{\hat\sigma i}$. The energy of the bound state and the parameter R are determined from Eq. (11) for $i \in$ TB. In the leading order in Δ, that is, neglecting corrections $O(\Delta^2/\varepsilon_F)$ to the energy, the characteristic equation coincides with Eq. (10) for the two-component function (13). Solving it for $U_0 = 0$ we find that all bound states have zero energy independent of normal state anisotropy. They exist if the gaps of incident and outgoing quasiparticles satisfy

$$\Delta_+\Delta_- > 0 \ , \qquad (14)$$

e.g., for $k_{y\mathrm{C}} < k_y < k_{y\mathrm{A}}$ and for $k_y > k_{y\mathrm{D}}$ and $k_y < k_{y\mathrm{B}}$ in Fig. 2. Taking into account the symmetry of the twin boundary it is easy to see that this condition coincides with the previously obtained $\Delta(\mathbf{k}_F, \infty)\Delta(\mathbf{k}_F, -\infty) < 0$. It is, however, opposite to the condition on the existence of surface bound states in a d-wave superconductor [14].

The boundary potential U_0 splits the degeneracy between even and odd states. For quasiparticles moving nearly perpendicular to the twinning plane, the dimensionless parameter $\alpha = U_0/\sqrt{2}v_{Fx} \sim U_0/\varepsilon_F$ is small. Bound states exist in the same region as in unperturbed case (14) and their energies acquire dispersion

$$E_{\mathrm{even,odd}} = \pm \frac{2\alpha\Delta_+\Delta_-}{|\Delta_+ + \Delta_-|} \ , \qquad (15)$$

which yields a finite width of zero-energy peak in the local density of states (4). The effect of the boundary potential is destructive for bound states with wave vectors $\mathbf{k}_\pm$ nearly parallel to the twin boundary, i.e., for bound states with $k_y > k_{y\mathrm{D}}$ and $k_y < k_{y\mathrm{B}}$ in Fig. 2. A weak barrier $U_0/\varepsilon_F \sim \Delta_s/\Delta_0$ is sufficient to destroy completely these bound states.

As a further check of the robustness of the midgap bound states, we have relaxed the condition of constant nearest-neighbors pairing amplitudes in the Hamiltonian and changed them near the twin boundary as shown in Fig. 1. This change models a space dependent gap on the discrete lattice and again does not affect energies of the bound states irrespective of the difference between Δ's and Δ''s.

The transmission of excitations by the twin boundaries, which is important for the heat conduction process at low temperatures, also has unusual features. In particular, for $T < \Delta_s$ the heat is carried to the twin boundary by low energy excitations with $\mathbf{k} \approx \mathbf{k}_\mathrm{A}$ in Fig. 2. For these quasiparticles $|\Delta_-| < E < |\Delta_+| \approx \Delta_s$. Let us consider such an electron-like state with $\mathbf{k} \approx \mathbf{k}_-^>$ approaching the boundary from the right. It cannot be reflected back into the twin as an electron with $\mathbf{k} \approx \mathbf{k}_+^>$, nor transmitted across the boundary as an electron with $\mathbf{k} \approx \mathbf{k}_-^<$, since the gap magnitude for the outgoing quasiparticles is $|\Delta_+| > E$. However, this electron can transform into a hole having $\mathbf{k} \approx \mathbf{k}_-^>$ and the same gap Δ_- but with the opposite group velocity (Andreev reflection [15]). In the case of zero barrier ($U_0 = 0$) the Andreev reflection is perfect (there is only an exponentially decaying wave in the left twin). The transmission of heat across the twin boundary must thus come from excitations with $E > \Delta_s$ and there will be a temperature dependent contribution to the thermal conductivity from the twinning planes of the form $\kappa_{\mathrm{TB}} \propto \exp(-\Delta_s/k_B T)$.

An extra potential U_0 on the twin boundary, however, opens up an additional scattering channel in which an incident electron-like quasiparticle transforms into an outgoing hole-like excitation with $\mathbf{k} \approx \mathbf{k}_+^<$ on the other side of the boundary (Fig. 2). It is this process of Andreev *transmission*, which will be responsible for the thermal conductivity across the twin boundaries in the low temperature limit. Interestingly, the boundary barrier U_0,

which causes reflection of the quasiparticles from the twin boundary in the normal state, allows transmission of the low-energy excitations in the superconducting state.

Finally, we comment on properties of bound quasiparticles for the time-reversal breaking superconducting state of the twin boundary [7]. These effects can be most easily understood on the basis of Eq. (1). We assume that the gap function has, in addition to (2), a small imaginary component of the s-wave harmonic $i\Delta_s f(x)$, $f(x)$ being an even function. The right-hand side of Eq. (1) contains in this case an extra term $-\Delta_s \tau_2 f(x)$. First-order energy corrections found by averaging this perturbation with respect to the unperturbed states (3) are nonzero and have opposite signs for ψ_+ and ψ_-. As a result, the bound state peak (4) in the local density of states shifts to finite energies, making possible to distinguish the two superconducting states on twinning planes in tunneling experiments. Condensation of bound states with a nonzero momentum produces also a local current flow parallel to the twin plane, which was derived in [7] in the framework of the Ginzburg-Landau theory.

In conclusion, the formation of electron bound states on twin boundaries is a general property of orthorhombic predominantly d-wave superconductors. Observation of a bound state peak in the local density of states on twinning planes in YBCO by means of scanning tunneling microscopy would be a direct confirmation of the presence of s-wave component in CuO_2 planes. Also, a novel process of Andreev transmission is responsible for thermal conductivity across the twin boundaries in the low temperature limit.

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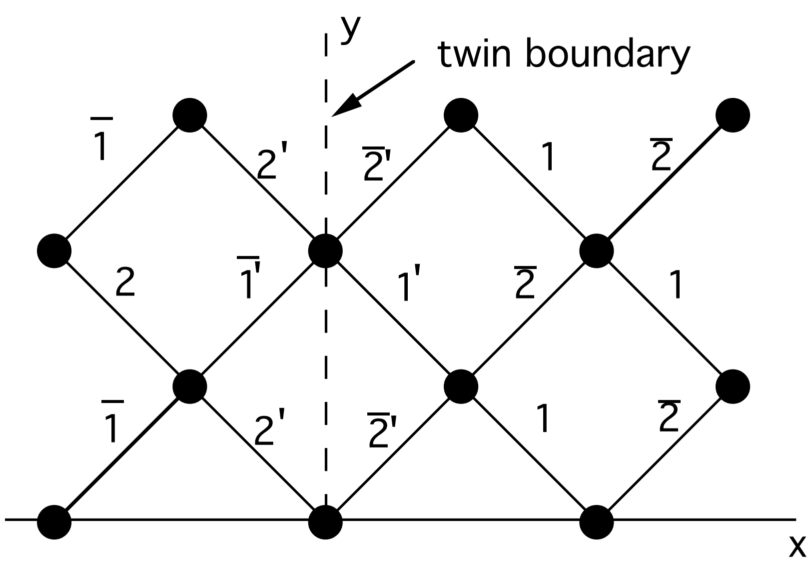
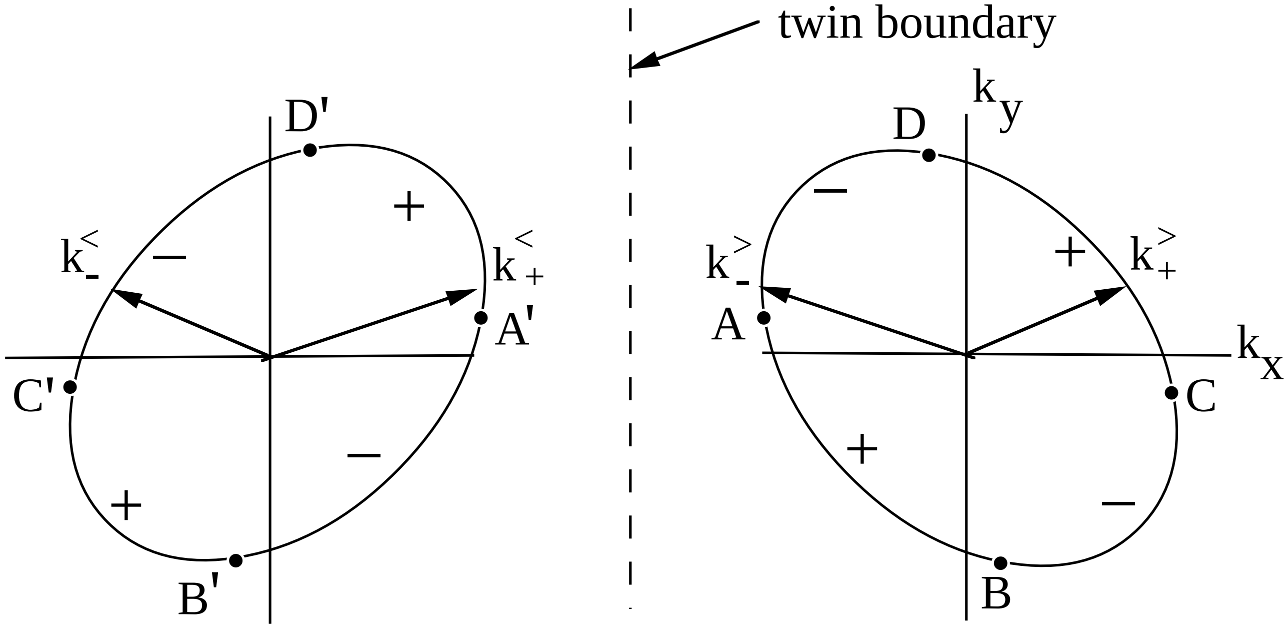
FIG. 1. Twin boundary and nearest-neighbor hopping and pairing amplitudes; $1 \equiv (t_1, \Delta_1/2)$, $\bar{1} \equiv (t_1, -\Delta_1/2)$, $1' \equiv (t_1, \Delta_1'/2)$, $\bar{1}' \equiv (t_1, -\Delta_1'/2)$, $2 \equiv (t_2, -\Delta_2/2)$ etc.

FIG. 2. Twin boundary and orthorhombic Fermi surfaces in the two twins. The capital letters A, B, ... denote the positions of nodes of the $d \pm s$ gaps. The sign of $\Delta(\mathbf{k})$ in the different regions on the Fermi surfaces is indicated as + or −.



y
twin boundary
$\bar{1}$
2'
$\bar{2}'$
1
$\bar{2}$
2
$\bar{1}'$
1'
$\bar{2}$
1
$\bar{1}$
2'
$\bar{2}'$
1
$\bar{2}$
x


twin boundary
D'
A'
B'
C'
D
A
B
C
$k_-^<$
$k_+^<$
$k_-^>$
$k_+^>$
k_y
k_x
+
−